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OH (8, 3) band emission from different excitation mechanisms

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Abstract In this paper following Bates-Nicolet, Breig and Krassovsky, the excitation mechanisms of OH(8, 3) band and its altitudinal variation of volume emission rate are presented. Empirical relations between emission rate and altitude are also obtained. It is shown that experimental curve for OH (8, 3) band intensity agrees fairly well with the theoretical values obtained from Bates-Nicolet mechanism

Keywords · Airglow, excitation mechanisms of OH (8, 3) Band

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The self-luminescence of upper atmosphere is known as airglow Ions, atoms and molecules are excited by absorbing solar energy. Different collisional processes are also responsible for the excitation processes. When they come down to ground state or intermediate lower energy state, they emit energy in the form of light. This is known as airglow.

Ions, atoms and molecules of the upper atmosphere are not visible to us. From the intensity of airglow emission line one can understand the physical properties and the state of atoms and molecules of the atmosphere.

OH band is one of the important emissions of airglow spectrum. The peak height of emission of OH band is around 90 Km. The proposed excitation mechanism of OH band are as follows :

A. Bates-Nicolet mechanism [1]

i) $O + O_2 + M \xrightarrow{K_1} O_3 + M$,

ii) $O_3 + H \xrightarrow{K_2} O_2 + OH^*(3.32\ ev)$,

iii) $OH^* \xrightarrow{A_{ul}} OH + h\nu$,

where $K_1 = 1.5 \times 10^{-34} \exp\left(\frac{445}{T}\right) cm^6\ S^{-1}$ [2] and $K_2 = 1.5 \times 10^{-12} \sqrt{T}\ cm^3\ S^{-1}$ [3].

B. Breig mechanism [4]

$$H + M + O_2 \xrightarrow{K_5} HO_2 + M,$$

$$HO_2 + O \xrightarrow{K_6} OH^* + O_2,$$

where $K_5 = 3.3 \times 10^{-33} \exp\left(\frac{800}{T}\right) cm^6\ S^{-1}$ [5] and $K_6 = 1.5 \times 10^{-12} \sqrt{T}\ cm^3\ S^{-1}$ [5].

C. Krassovsky mechanism [6]

$$O_2 + O + M \xrightarrow{K_3} O_3 + M,$$

$$O + O_3 \xrightarrow{K_7} O_2^* + O_2^*,$$

$$O_2^* + H \xrightarrow{K_4} OH^* + O.$$

where $K_3 = 1.5 \times 10^{-32}\ cm^6\ S^{-1}$ and $K_4 = 10 \times 10^{-10}\ cm^3\ S^{-1}$ [7] $K_1, K_2, K_3, K_4, K_5, K_6$ and K_7 are reaction rate constants.

The purpose of this paper is to find the probable excitation mechanism of OH bands.

Volume emission rate from Bates-Nicolet mechanism :

From Bates-Nicolet excitation mechanism

$$\frac{d[O_3]}{dt} = K_1[O][O_2][M] - K_2[O_3][H].$$

At the steady state, $\frac{d[O_3]}{dt} = 0$;

hence $[O_3] = \frac{K_1[O][O_2][M]}{K_2[H]}$.

The rate of formation of OH* is given by :

$$n(OH^*) = K_2[O_3][H]$$

$$= K_2 \times \frac{K_1[O][O_2][M]}{K_2[H]} \times [H]$$

$$= K_1[O][O_2][M].$$

So the production of OH* depends on the concentration of atomic and molecular oxygen, hence on Ozone concentration. The formation of OH* is independent of hydrogen. So hydrogen acts as a catalyst for the above process.

In the mixed atmospheric region, the quenching by O, O_2 and N_2 will be important. The quenching reactions are as follows :

$$OH^* + O_2 \xrightarrow{l_{O_2}} OH + O_2 ,$$

$$OH^* + N_2 \xrightarrow{l_{N_2}} OH + N_2 ,$$

$$OH^* + O \xrightarrow{l_O} OH + O ,$$

where l_{O_2}, l_{N_2} and l_O are quenching rate constants due to O_2, N_2 and O respectively and their numerical values are given below :

$$l_{O_2} = 1.0 \times 10^{-14} \text{ cm}^3 S^{-1} \text{ [8]}$$

$$l_{N_2} = 3.6 \times 10^{-15} \text{ cm}^3 S^{-1} \text{ [8]}$$

$$l_O = 4 \times 10^{-11} \text{ cm}^3 S^{-1} \text{ [9]}$$

The volume emission rate of OH (8, 3) band considering all the important quenching factor is given by

$$Q_{OH^*} = \frac{A_{8,3} K_1 [O][O_2][M]}{\sum A_{vv'} + (l_O[O] + l_{O_2}[O_2] + l_{N_2}[N_2])} ,$$

where $A_{vv'}$ is the Einstein transition probability from vibrational level v to v'.

$$A_{8,3} = 0.0296 \text{ s}^{-1}$$

$$\sum A_{vv'} = 13.5 \text{ [10].}$$

From the number densities of N_2, O_2 and O [11] shown in Table 1, the volume emission rates of OH(8, 3) band at different altitudes are calculated and shown in Figure 1. An empirical relation is best fitted with this curve having the form

$$Q_{OH(8,3)} = K \exp [-b (h - h_{max})^2] \qquad (1)$$

where $K = 1659.4759$,

$b = 0.0184$,

and h_{max} corresponds to the altitude of maximum volume emission rate of OH(8, 3) band.

The intensity is calculated from the volume emission rate curve by the following formula :

$$I = \tfrac{1}{2} \times \text{peak emission rate} \times \text{layer thickness}$$

$$= \tfrac{1}{2} \times 20 \text{ km.} \times 2.1463 \times 10^3$$

$$= \tfrac{1}{2} \times 20 \times 10^5 \times 2.1463 \times 10^3 \text{ cm} \times \text{cm}^{-3} S^{-1}$$

$= 21.463 \times 10^8 \text{ cm}^{-2} S^{-1}$

$= 21.463 \times 10^3 R$

$= 21.463 KR.$

Table 1. Calculated volume emission rates from different excitation mechanism

Altitude (KM)	Bates-Nicolet $Q_{OH^*} \times 10^{-3}$ (cm^{-3} Sec^{-1})	Breig $Q_{OH^*} \times 10^{-3}$ (cm^{-3} Sec^{-1})	Krassovsky $Q_{OH^*} \times 10^{-3}$ (cm^{-3} Sec^{-1})	Experimental intensity $\times 10^{-3}$ (KR)
75	0 5011	5 89	4.69	1.07
76	0 8059	15 37	7 56	1 11
77	1 1530	24 33	10.81	1 25
78	1.1536	25 87	10.81	1.60
79	1 6447	19.12	15 41	2.23
80	1 2419	11 09	11 64	3 57
81	1 9274	8.18	20 43	6 00
82	2.1463	5 75	20 12	8 75
83	2.0243	3 90	18 96	11.00
84	1 6737	2 45	15 69	13 00
85	1 2049	1 40	11 29	13 57
86	1.1990	0 97	12 94	16 60
87	1 1067	0 64	10 37	17.00
88	0 8657	0 42	8 12	16 34
89	0.6388	0 24	5 98	13 75
90	0 4044	0 13	3.79	11 00
91	0 3257	0 08	3 06	8 30
92	0.2389	0 05	2 24	5 71
93	0 1819	0 03	1.70	2 85
94	0 1275	0 02	1 19	0 80
95	0 09116	0 01	0 85	0 357

Volume emission rate from Breig mechanism :

From Breig mechanism

$$\frac{d[HO_2]}{dt} = K_5[H][M][O_2] - K_6[\bar{H}O_2][O].$$

At the steady state, $\frac{d[HO_2]}{dt} = 0$;

hence, $[HO_2] = \frac{K_5[H][M][O_2]}{K_6[O]}$

The rate of formation of OH* is given by

$$n(OH^*) = K_6[HO_2][O] = K_6 \times \frac{K_5[H][M][O_2]}{K_6[O]} \times [O] = K_5[H][M][O_2].$$

OH* formation is hence dependent on atomic hydrogen concentration.

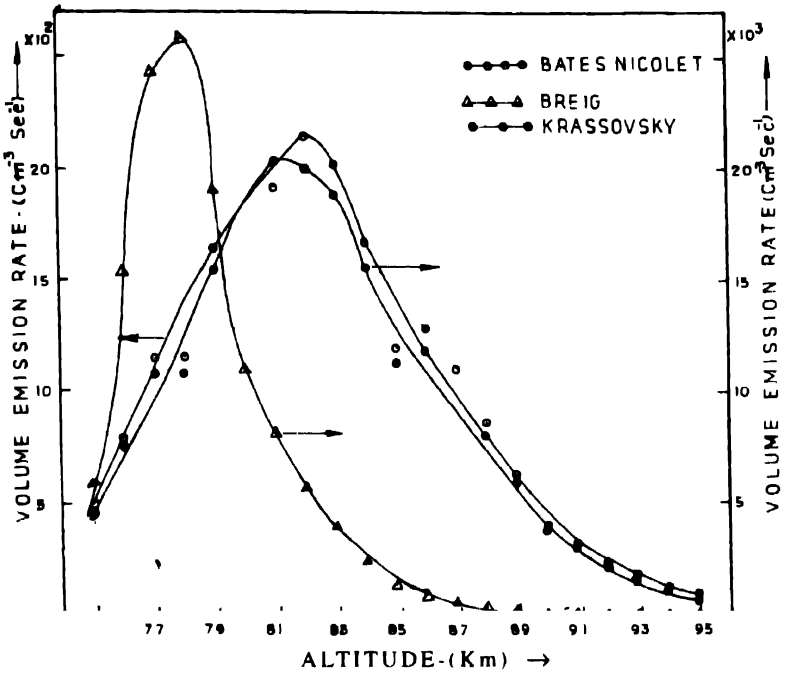

Figure 1. Altitudinal distribution of OH (8, 3) band

The volume emission rate of OH(8, 3) band considering all the important quenching factors is given by

$$Q_{OH^*} = \frac{A_{8,3}\, K_5[H][M][O_2}{\Sigma A_{vv'} + (I_O[O] + I_{O_2}[O_2] + I_{N_2}[N_2]}$$

From the number densities of H, O_2 and N_2 shown in Table 1, the volume emission rate of OH (8, 3) at different altitudes are calculated and shown in Figure 1. The empirical equation 1 has been fitted with this curve. Hence, the values of K and b are 9.836×10^3 and 0.0264 respectively and the value of h_{max} is 78 km. The intensity is 103.48 KR.

Volume emission rate from Krassovsky mechanism :

From Krassovsky mechanism

$$\frac{d[O_3]}{dt} = K_3[O][O_2][M] - K_7[O][O_3]$$

and

$$\frac{d[O_2^*]}{dt} = K_7[O][O_3] - K_4[O_2^*][H].$$

At the steady state, $\frac{d[O_3]}{dt} = 0$, $\frac{d[O_2^*]}{dt} = 0$;

Hence, $$[O_3] = \frac{K_3}{K_7}[O_2][M].$$

$$[O_2^*] = \frac{K_7[O][O_3]}{K_4[H]}$$

$$= \frac{K_7}{K_4} \times \frac{[O]}{[H]} \times \frac{K_3}{K_7}[O_2][M]$$

$$= \frac{K_3}{K_4} \times \frac{[O][O_2][M]}{[H]}.$$

The rate of formation of OH* is

$$n(OH^*) = K_4[O_2^*][H]$$

$$= K_4 \times \frac{K_3[O][O_2][M]}{K_4[H]} \times [H]$$

$$= K_3[O][O_2][M].$$

Hence OH* formation is also dependent on concentration of atomic hydrogen.

The volume emission rate of OH(8, 3) band is

$$Q_{OH}^* = \frac{A(8,3)\, K_3[O][O_2][M]}{\sum A_{vv'} + (l_O[O] + l_{O_2}[O_2] + l_{N_2}[N_2])}.$$

The volume emission rate is calculated with the above equation and shown in Figure 1. The empirical eq. (1) is also fitted with this curve. The values of K, b and h_{max} are 15.297×10^3, 0.0154 and 81 km respectively. The intensity is calculated and it is 219.35 KR.

From correlation coefficient and coefficient of variations (Table 2), it appears that Bates-Nicolet mechanism and Krassovsky mechanism are close to experimental curve of Evans *et al.*

Table 2. Calculated correlation coefficients, coefficient of variation and intensities

Mechanisms	Bates-Nicolet mechanism	Breig mechanism	Krassovsky mechanism	Experimental
Correlation coefficient between volume emission rate with experimental intensity of OH(8, 3) band	0.274	−0.5302	0.272	–
Coefficient of variation C.V. $= \frac{\sigma}{\bar{x}} \times 100\%$	64.09%	135.61%	65.22%	78.13%
Intensity	21.46 KR	103.48 KR	219.35 KR	17 KR

[12]. But the calculated intensity from different mechanisms shows that Bates-Nicolet mechanism is very close to the experimental result. So Bates-Nicolet mechanism is the appropriate excitation process of OH omission.

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